- Objective:

A new **N**ano**E**lectronic **MO**deling Tool

» Incorporate the best of existing simulators NEMO-1D, NEMO-3D, NEMO-3D-Peta and OMEN

» General atomistic structures

» Long-term development, sustainability

- Result:

» Strain and Phonons (VFF method)

» Electronic structure (tight-binding)

» Schroedinger-Poisson solver

» Quantum transport (NEGF, open-boundary wavefunctions)

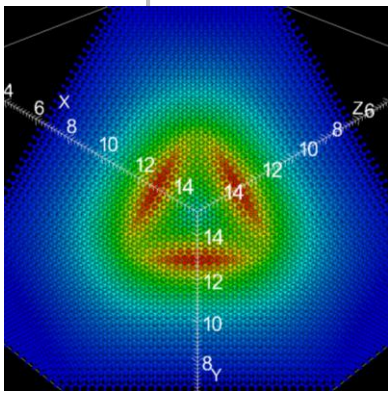
» Spinoff nanoHUB apps

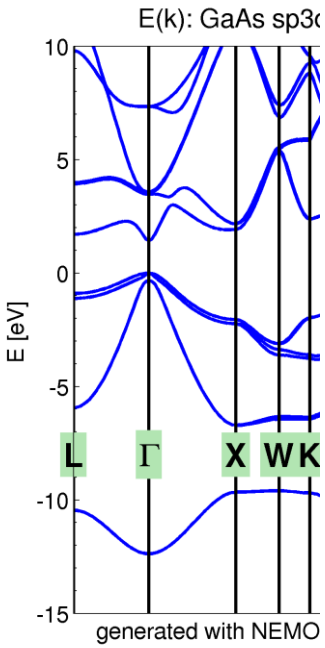
- Approach:

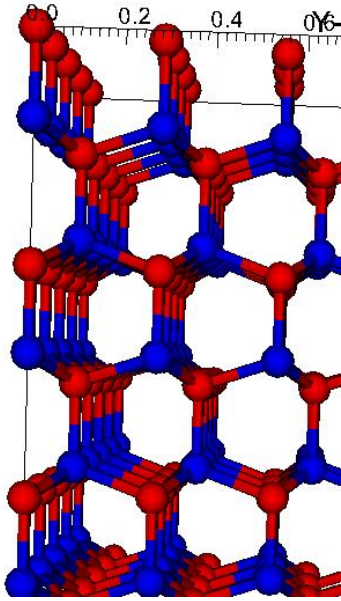
» C++, MPI

» Leverage mature OS packages: PETSc, SLEPc, libmesh, VTK, …

» **Teamwork:**
→ 4 post doc core team (Steiger, Povol., Kubis, Park)
→ >5 grad students & other post docs involved







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